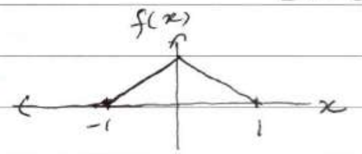
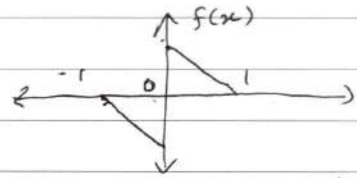
ADVANCED MATHEMATICAL METHODS FOR CHEMISTRY - QUIZ 8

SOLUTIONS

1 

Clearly even functions - so only nonzero cosine terms (c)

2 

Odd function, so $A_0 = 0$ (d)

3 $f(x) = 4\sin 3x + (2\cos x + 2i\sin x)\cos 2x$

$= 4\sin 3x + \cos 3x + \cos x + i\sin 3x - i\sin x$

$\underline{A_3 = 1}$ coefficient $= 1$ (a)

4 $A\cos 2x = \frac{A}{2}e^{2ix} + \frac{A}{2}e^{-2ix}$

$p = 2\pi$ or -2π (c)

5 $\psi(x) = A\sin kx + B\cos kx$ $\psi(1) = 0 \Rightarrow A\sin k + B\cos k = 0$

$\psi(3) = 0 \Rightarrow A\sin 3k + B\cos 3k = 0$

$A(\sin 3k - \sin k) + B(\cos 3k - \cos k) = 0$

$A\frac{(\sin 4k - \sin 2k)}{2} + B\frac{(\cos 2k - \cos 4k)}{2}$

$2A\cos 2k\sin k - 2B\sin 2k\sin k = 0$

$\Rightarrow 2\sin k\,(A\cos 2k - B\sin 2k) = 0$ —①

Similarly $A(\sin 3k + \sin k) + B(\cos 3k + \cos k) = 0$

$2\cos k\,(A\sin 2k + B\cos 2k) = 0$ —②

say $\sin k = 0 \Rightarrow k = n\pi \Rightarrow \sin 2k = 0$ $\sin 3k = 0$

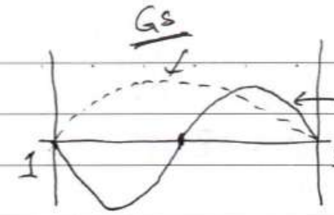
$\psi(1) = B\cos k \Rightarrow B = 0$

$\psi = A\sin(n\pi x)$ $n = 1, 2, 3 \ldots$

Other case $\cos k = 0$ $k = (2n+1)\frac{\pi}{2}$

Clearly only choice (c) fits. However, this is not ground state

Since



$\sin(\pi x)$ since Length of box = 2

Answer (d)

[6] $y'' - 2xy' + 2ny = 0$

Let $r(x) = e^{-x^2}$

$$y'' e^{-x^2} - 2x \cdot e^{-x^2} y' + 2ny\, e^{-x^2} = 0$$

$$\left[e^{-x^2} y'\right]' + \left[0 + e^{-x^2} \times 2n\right] y = 0$$

Answer (c)

[7] $$\int_{-\infty}^{\infty} H_v(x)\, H_{v'}(x)\, e^{-x^2}\, dx = 0 \quad \text{unless } v = v' \qquad (a)$$

[8] $$(1-x^2)\, y'' - 2xy' + \left\{ l(l+1) - \frac{m^2}{1-x^2} \right\} y = 0$$

$$\left[(1-x^2)\, y'\right]' + \left[l(l+1) \times 1 - \frac{m^2}{1-x^2} \right] y = 0$$

$$\lambda(x) = 1 \qquad -(c)$$

[9] $$\int_{-1}^{1} P_1(x)\, P_2(x)\, dx = 0 \qquad (b)$$

[10] Let $r(x) = e^{-x}$

$$x y'' e^{-x} + e^{-x} y' - x e^{-x} y' + n y e^{-x} = 0$$

$$\left(x e^{-x} y'\right)' + n e^{-x} y = 0$$

Answer (c)